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Electronic correlations in $FeSb_2$: a QSGW+DMFT investigation
WALBER HUGO DE BRITO, SANGKOOK CHOI, Brookhaven National Laboratory, GABRIEL KOTLIAR, Brookhaven National Laboratory and Rutgers University — Optical conductivity measurements of iron antimonide ($FeSb_2$) have shown that a large spectral weight redistribution takes place when the material is cooled down to 10 K [1]. On the theoretical side, density functional theory and GW calculations are known to predict metallic and insulating phases with a too large band gap, respectively. These findings suggest that electron correlations are relevant for the gap formation in $FeSb_2$ and that a theoretical description beyond a many-body perturbation theory is required. In this study we investigate from an *ab initio* perspective the role played by electron correlations on the electronic properties of $FeSb_2$. With our combined quasiparticle self-consistent GW (QSGW) and dynamical mean field theory (DMFT) calculations we reveal that many-body correlation effects lead to a temperature dependent gap renormalization. In particular, our calculations indicate that the dynamical behavior of the real parts of valence and conduction self-energies is of great importance to the gap formation in $FeSb_2$. [1] Phys. Rev. B **82**, 245205 (2010).

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